

Propyl carbamate

627-12-3 | DTXSID7060833

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 192 °C

Global applicability domain: Outside

Local applicability domain index: 6.87e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propyl carbamate</div> <div>Measured: 196</div> <div>Predicted: 192</div>	<div>Image not found</div> <div>Isopropyl carbamate</div> <div>Measured: 183</div> <div>Predicted: 187</div>	<div>Image not found</div> <div>Carbamic acid, 2-methylpropyl ester</div> <div>Measured: 207</div> <div>Predicted: 199</div>
<div>Image not found</div> <div>Urethane</div> <div>Measured: 185</div> <div>Predicted: 184</div>	<div>Image not found</div> <div>N-Methylcarbamic acid, ethyl ester</div> <div>Measured: 170</div> <div>Predicted: 176</div>	